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ABSTRACT

Listings of suggested topics aimed at helping university and college faculties plan courses in the main areas of the chemistry curricula are provided. The suggestions were originally offered as appendices to the American Chemical Society's (ACS) Committee on Professional Training's 1983 guidelines for ACS-approved schools. The course data included in the listings attempt to cover both some of the similarities and some of the breadth of current offerings in undergraduate chemistry programs. Many of the outlines and questions were assembled with help from divisions of the ACS as well as from persons with wide curricular contacts. The areas of the chemistry curriculum discussed are: (1) analytical chemistry; (2) biochemistry; (3) chemical health and safety; (4) chemical information retrieval; (5) computers in chemistry; (6) industrial chemistry; (7) inorganic chemistry; (8) organic chemistry; and (9) polymer chemistry. (JN)

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Chemistry Curricula. Course Suggestions

American Chemical Society
Committee on Professional Training
Washington, DC

1984

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ANALYTICAL CHEMISTRY

(Prepared with the Help of the ACS Division of Analytical Chemistry)

A sequence of courses designed to cover modern analytical chemistry at the undergraduate level should present an integrated view of the theories and methods for solving a variety of real problems in chemical analysis. Students should receive a coherent and progressive treatment of the various aspects of problem definition, physiochemical operations, and data evaluation. The problem-oriented role of chemical analysis should be emphasized throughout the student's experience. (The appendix material for Computers in Chemistry should also be consulted. Additionally, the Analytical Chemistry Subcommittee of the Division of Chemical Education Curriculum Committee has prepared an extensive document with performance objectives for analytical chemistry.)

I. In addition to a firm foundation in basic chemical reactions involving analytes and ordinary analytical reagents, adequate coverage of modern analytical chemistry should include:

   A. Distinction between qualitative and quantitative goals of determinations
   B. Choice of experimental designs
   C. Sampling methods for all states of matter
   D. Sample preparation and derivatization procedures
   E. Availability and evaluation of standards
   F. Standardization methodology
   G. Theory and methods of separation
   H. Physico-chemical methods of measurement
   I. Fundamental characteristics of instruments, including recording devices, and data acquisition options
   J. Comparison and critical selection of methods for both elemental and molecular determinations
   K. Optimization techniques for various aspects of analysis
   L. Methods of data evaluation

II. Individual topics should be presented in the framework of a systematic approach which emphasizes functional roles, facilitates comparison of performance characteristics, and provides a pattern the student can use to understand related topics not included in formal course work. The courses should integrate chemical and instrumental concepts; they should include examples from inorganic, organic, and biological chemistry; they should emphasize the importance of kinetic and equilibrium aspects of both chemical and physical processes; and they should emphasize interactions and resulting interdependencies among different steps in the analytical process. The courses should include discussion of methods used to optimize performance characteristics such as selectivity, sensitivity, uncertainty, and detection limits. They should examine the trade-offs that are made among these performance characteristics and practical considerations, such as time and cost, which are always associated with real problem--e.g. an industrial process, a clinical problem, or an experiment performed in outer space.

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III. Some topics in modern analytical chemistry may not require a thorough background in physics and/or certain areas of physical chemistry. Accordingly, these topics may be introduced in lower division courses. However, in order to achieve finally the desired depth and breadth in modern analytical chemistry at the undergraduate level, the more advanced topics in theory and methods should have as prerequisites calculus-based physics, basic inorganic and organic chemistry, an upper-level treatment of structure-energy relationships, fundamentals of thermodynamics and electrochemistry, and basic chemical dynamics.

IV. While all ares of chemistry utilize the concepts and techniques referred to above, it is the responsibility of the analytical chemist(s) to coordinate and reinforce their presentation. The student should emerge from an undergraduate program of studies in analytical chemistry with the following competencies:

A. Define clearly problems of chemical analysis. Is the information required of a qualitative or quantitative nature? If quantitative, what are the acceptable accuracy and precision limits? Is it an elemental or molecular determination? What are the chemical and physical properties unique to the analyte and what matrix effects should be considered in designing the experiments? How is data to be evaluated, interpreted, and optimized?

B. Select wisely a method, or methods, to achieve the goals in A. This implies that the student should understand the chemical and instrumental options available for both elemental and molecular determinations, as well as equilibrium and kinetic processes. The student must understand the basic chemical reactions which will be involved in sample acquisition and preparation and separations. The student must know how to eliminate or compensate for interferences. The student must recognize the critical response parameters for each phase of the determination and must be able to identify the sources of error.

C. Utilize the proper methods of statistical evaluation of data, including validation and optimization techniques. A thorough understanding of standardization methodology is prerequisite, as is knowledge of the sources of errors, instrumental and chemical.

D. Understand the theory and operational principles of the fundamental components of instrumentation for:

1. Spectrometry

a. Atomic (AE, AA, X-ray)
b. Molecular (UV-Vis, IR, Fluorescence)
c. Mass

2. Separations

   a. GC
   b. LC

3. Magnetic Resonance

   a. NMR
   b. EPR

4. Electroanalytical Methods

   a. Potentiometric (pH, ISE)
   b. Voltammetric
   c. Coulometric
   d. Conductimetric

5. Thermal Methods (Thermometric Titrations, DTA, DSC)

6. Radiochemical Methods (Activation Analysis, LSC)

7. Computerized Data Acquisition

8. Recording Devices and Electronic Testing

BIOCHEMISTRY

If biochemistry is not presented as a separate course in the curriculum, then fundmental topics drawn from biochemistry must be covered in the core curriculum, particularly in organic and physical chemistry. Item I below is a minimal list of fundamental topics. Following coverage of these fundamental topics a rigorous survey course in biochemistry, making use of quantitative concepts involving kinetics, thermodynamics and solution properties of marcomolecules might serve as an advanced course (item II). Especially recommended, however, more focused courses that provide depth in one or a few specialized areas (item III). A survey course in biochemistry to emphasize the metabolic significance of the fundamental topics in biochemistry covered in the core curriculum should be a prerequisite for the specialized courses.

I. Fundamental Topics in Biochemistry

- A. Chemistry of amino acids and peptides
- B. Introduction to protein structure and enzyme mechanisms
- C. Chemistry of nucleotides and nucleic acids
- D. Introduction to structure of DNA and RNA
- E. Chemistry of lipids
- F. Introduction to structure of biomembranes and plasma lipoproteins
- G. Chemistry of carbohydrates

II. Topical List of a Rigorous, Physical Chemistry-Based Biochemistry Survey Course

- A. Amino acids, peptides, proteins
- B. Enzymatic kinetics and regulation
- C. Carbohydrates
- D. Nucleotides and nucleic acids
- E. Lipids
- F. Structure and function of biomembranes and plasma lipoproteins
- G. Solution properties of macromolecules
- H. Metabolism
  - -- Bioenergetics
  - -- Carbohydrates, amino acids, lipids, nucleic acids
- I. DNA,RNA and protein synthesis
- J. Recombinant DNA
- K. Complex carbohydrates, glycoproteins
- L. Muscle and connective tissue proteins
- M. Hormones and receptors
- N. Molecular endocrinology
- O. Neurochemistry
- P. Immunochemistry

III. Specialized Areas of Biochemistry Suitable for an Advanced Course

- A. Enzymatic catalysis
- B. Molecular genetics
- C. Recombinant DNA technology

D. Solution properties (physical and chemical) of biological macromolecules
E. Complex carbohydrates and glycoproteins
F. Immunochemistry
G. Neurochemistry
H. Chemistry of hormones and receptors
I. Biological membranes

IV. TYPICAL SCIENCE CURRICULUM FOR A BACHELOR'S DEGREE IN BIOCHEMISTRY*

(Approved by the Council of the American Society of Biological Chemists, Autumn 1981)

		Number of Semesters
BIOCHEMISTRY	Prerequisites: 1 year	2-3
BIOCHEMISTRY LABORATORY	of organic chemistry	1-2
CHEMISTRY		
General	(includes inorganic)	2
Organic		2
Physical	(based on calculus)	2
Analytical		1
BIOLOGY		
Genetics		1
Microbiology		1
Cell biology		1
Advanced course (e.g., animal or plant physiology, immunology, virology)		1
MATHEMATICS		
Through integral calculus		
Additional courses in statistics or computer science are encouraged		2-3
PHYSICS		2

Opportunities for individual research are desirable

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* This is <u>not</u> a CPT-approved curriculum. (Under-represented, for example, are the areas of analytical and inorganic chemistry.) It is included to help clarify differences between degrees in chemistry and biochemistry, and for the information of faculty advisors and students, particularly at those institutions where many, perhaps most, chemistry majors are headed for careers in medicine or related fields. A student who has completed this biochemistry curriculum may be within a course or two of having a certifiable degree in chemistry.

CHEMICAL HEALTH AND SAFETY

(Prepared with the Help of the ACS Division of Chemical Health and Safety)

Proper chemical health and safety practices on campus are not limited to the use of chemicals in chemistry laboratories, lecture experiments, and demonstrations in chemistry classrooms. Consider those departments that instruct in art, physics, geology, psychology, theatre, engineering, agriculture (to name a few of the many other chemical users), as well as maintenance, janitors, security (and other service personnel) and not forgetting office workers -- all are involved in the use of chemicals. However, given the purposes of this appendix to the CPT Guidelines, these remarks will only pertain to certain chemical health and safety policies and practices within the chemistry department of an academic institution.

The ACS Division of Chemical Health and Safety (DIVCHAS) offers for consideration by chemistry faculty and institution administrators this check list of items in decreasing order of importance. At the minimum, these matters should be addressed in order to reduce the probability of harm to students when chemicals are used and in order to insure that students are instructed in the safe and healthy use of chemicals:

1. There should be a formal policy statement affirming the importance of proper chemical health and safety practices, signed by the current president of the institution, or, preferably, the chairman of the board of trustees. This statement (or derivative statements) should establish clear lines of responsibility and enforcement authority, with sanctions and appeal procedures, etc. It should include provision for an annual budget line item for improvement of chemical health and safety practices within the institution as a whole and/or within each separate administratively distinct entity that uses chemicals.

2. The institution-wide policy should be implemented in a <u>practical</u> "Chemistry Safety and Health Operations Manual" which mandates detailed procedures for the requisitioning, inventorying, handling, use, storage and disposal of chemicals and the precautions to be followed in the use of associated equipment and apparatus.

3. There should exist documentary evidence, such as minutes of chemistry faculty (or faculty committee) meetings, of annual (or more frequent) reviews of departmental policies toward, and the efficacy of their implementation in, the practice and the teaching of chemical health and safety. For example, the relevant documents might show a recent consideration of the institution of a credit course on chemical health and safety as a new offering, or, if already existing, a review of the content and conduct of that course and its application by students and faculty in other chemistry courses.

4. If it has been determined that a formal course is inappropriate, there should exist similar evidence (such as recent meeting minutes) describing other ways in which students will be instructed in these matters. Such evidence should show that the four year chemistry curriculum is intended to inculcate students' competence in, and their habitual practice of, the principles of chemical health and safety.

5. There should be centrally located as well as departmental library holdings of publications dealing with chemical health and safety, together with evidence that these are used by both faculty and students.

6. As is well known, faculty promotion and tenure procedures generally do not include considerations of a candidate's interest or competence in chemical health and safety as an important criterion in the deliberative processes. Until these matters are included, real progress in the improvement of instruction in and the practice of chemical health and safety will necessarily be slow or non-existent. DIVCHAS recognizes that incorporation of such criteria into the tenure and promotion milieu is controversial and for this reason places this matter in sixth (least important) position. In a sense, DIVCHAS believes that it should be the first, and perhaps the only, item. DIVCHAS recommends that all academic institutions consider that a chemistry faculty member's interest and competence in instructing students in chemical health and safety should be one of the criteria that determines promotion and tenure.

Selected References for library and/or personal holdings:

Safety in the Academic Laboratory, ACS Council Committee on Chemical Safety, ACS, Washington, DC, 1984.

Safety in the Chemical Laboratory, Vols. 1 - 4, Norman Steere and Malcolm Renfrew, Editors, DIVCHED, 238 Kent Road, Springfield, PA 19064, 1967, 1971, 1974, 1980, resp.

Laboratory Safety Guidelines, James A. Kaufmann, 101 Oak Street, Wellesley, MA 02181, 1981.

Hazards in the Chemical Laboratory, 3rd edn., Leslie Bretherick, Editor, The Chemical Society, Burlington House, London W1V 0BN, 1981.

Safety and Accident Prevention in Chemical Operations, 2nd edn., Howard H. Fawcett and William H. Wood, Editors, John Wiley and Sons, NY, 1982.

Handbook of Reactive Chemical Hazards, 2nd edn., Leslie Bretherick, Butterworths, Boston, 1979.

Safety, module IX of a TV tape series, David Brooks, Editor, Project Teach, University of Nebraska, Lincoln, NE 68588, 1980.

Patty's Industrial Hygiene and Toxicology, Vols. 2A, 2B, 2C, 3rd rev. edn., G. D. Clayton and F. E. Clayton, Editors, Wiley Interscience, NY, 1981 and 1982.

Material Safety Data Sheets, for every chemical used -- obtained from the manufacturers.

Fire Protection for Laboratories Using Chemicals, Code 45, National Fire Protection Association, Quincy, MA 02269, 1982.

Fire Protection Guide on Hazardous Materials, 7th edn., Ibid., 1978.

Guide to Safe Handling of Compressed Gases, Matheson Gas Products, Seacaucus, NJ 07094, 1983.

Best Safety Directory, Vols. 1 and 2, A. M. Best Co., Oldwick, NJ 08858, revised frequently.

Catalog, Laboratory Safety Supply Co., Janesville, WI 53547, revised frequently.

The following articles, some provocative, some informative, will be useful. (All are from the Journal of Chemical Education unless otherwise stated.):

A safety exam, 55, A129 and A193 (1978); safe storage, 59, A159 (1982); assessing hazards, 59, A265 (1982); toxic vapors in the laboratory, 59, A385 (1982); risk/benefit balance, 59, 954 (1982); waste disposal, 60, A81 and 490 (1983); labels, 60, A141 (1983); safety and health dos and don'ts, 60, 1067 (1983); effects of exposure to toxic vapors, J. Occ. Med., 21, 413 (1979); corrosive effects, Toxic and Appl. Pharma., 42 (2) 417 (1977).

CHEMICAL INFORMATION RETRIEVAL

(Prepared with the Help of the ACS Division of Chemical Information)

A student who intends to become a practicing chemist, or who will use chemistry in allied fields of science and medicine, should know how to use the chemical literature effectively and efficiently. Guidelines for instruction in chemical information retrieval for chemistry majors are given in this appendix, including an outline of course content, the level of ability desired, and suggestions as to ways in which library skills may be imparted.

I. Topics and Skills

A. A student graduating with an ACS certified degree in chemistry should have a demonstrable understanding of the general content and organization of:

1. Chemical Abstracts
2. Other principal secondary sources, e.g., Beilstein, Current Contents, Index Chemicus, Science Citation Index, etc.
3. Standard reference works, e.g., Handbook of Chemistry and Physics, Gmelin, Mellor, Landolt-Bornstein, etc.
4. Primary literature sources
5. Computerized chemical databases, e.g., Chemical Abstracts Services CA file and Registry file

B. In order to use the primary and secondary literature effectively, the student should be familiar with:

1. The organization of the chemistry library
2. Techniques of manual literature searching
3. Techniques of online, interactive literature searching

C. Students should be able to:

1. Efficiently locate chemical and physical properties of substances, including their spectra.
2. Efficiently locate references for the synthesis or reactions of desired compounds or classes of compounds.
3. Efficiently locate references to a desired type of chemical transformation.
4. Identify the CAS registry number of compounds
5. Complete a comprehensive subject search. Utilize CA subject indexes and Index Guide.
6. Compile a complete bibliography of an author's publications.
7. Locate recent review articles on a subject.
8. Utilize a variety of methods to stay up-to-date on a subject.
9. Know the importance of patents and be able to search for patents on a subject.
10. Know about the availability and contents of relevant computerized databases (bibliographic and nonbibliographic) and understand the basic techniques of online searching. (It is not anticipated that proficiency at online searching will be achieved, but the ability to interact productively with an information specialist is expected.)

D. Proficiency in chemical information retrieval should be acquired through formal instruction. In particular, Chemical Abstracts has become sufficiently complex that its use can no longer be easily self taught. Instruction can be achieved in the following ways:

1. Through a course dedicated to the subject of chemical information retrieval. A dedicated course of this kind can be greatly enhanced through library assignments from other courses.

2. Through integration into other chemistry courses, such as:

   a. laboratory courses, from sophomore through senior year, as assignments require library work
   b. upper division courses
   c. seminars
   d. independent study
   e. research
   f. combination with a course in technical writing

3. Through coordination and monitoring of each student's satisfactory achievement, preferably by one faculty member or librarian.

II. Implementation of Library Instruction

A. Faculty and librarians who are interested in developing instruction in chemical information retrieval but who lack the time or teaching aids to design such a course may contact the ACS Chemical Information Division, Education Committee, for suggestions and help. Course outlines, lists of texts on information retrieval and literature searching, lists of audio courses, library exercises, lists of online services and manuals, and other helpful guidelines may be obtained, if required, from the Chemical Information Education Committee.

B. Colleges that are unable to subscribe to Chemical Abstracts, including the volume indexes, because of cost are encouraged to take advantage the College Program offered by Chemical Abstracts. Reliance on neighboring institutions for access to Chemical Abstracts does not provide the environment in which students learn to use the literature as an integral part of their curriculum.

C. Primary journals, abstract journals, standard reference works, data compilations, monographs are crucial components of a library collection in chemistry. Information on a balanced collection to support undergraduate programs may be found in the 1982 revision of the "Guidelines and Suggested Title List for Undergraduate Libraries" prepared by the ACS Division of Chemical Education.

D. Online literature searching is a powerful tool which is rapidly becoming indispensible to the chemist. Successful literature searching requires a solid understanding of the databases being searched. Educational files that permit demonstration of computerized data bases are available online at relatively low cost. It is most desirable that more of these data bases be made available to educational institutions in the near future. In this regard, Chemical Abstracts Services now offers their complete CA file and Registry file at reduced rates to colleges and universities on a monthly or yearly subscription basis. Hands-on experience at online interactive searching is made possible through these files, which can be accessed readily through a variety of terminals including Apple, IBM, Osborne, and other microcomputers.

COMPUTERS IN CHEMISTRY

(Prepared with the Help of the ACS Division of Computers in Chemistry)

Computers and computer-aided technology have become an integral part of many aspects of modern chemistry. Interactions of chemists with computerized information retrieval services, computer-aided problem analysis, automated analytical instrumentation, and expanding applications of chemometrics are becoming more and more prevalent. The great versatility and availability of microcomputers makes the cost of hardware and software a minimum barrier to incorporation of computer-based instruction and enhancement into the undergraduate curriculum.

I. TOPICAL OUTLINE

The topics and concepts listed represent goals in a rapidly developing field. They range from introductory topics already an integral part of many programs to other topics where recent developments are changing so fast that courses will have to be updated regularly as development occurs. The appendix material for Analytical Chemistry and Chemical Information Retrieval should also be consulted. For example, note that items such as C and D may be appropriate for advanced instrumental courses.

A. Introduction: capabilities and properties of digital computers; accuracy and precision; significance of numbers; error accumulation; the floating-point number system; design of algorithms; selection of appropriate hardware and software resources for a particular application (mainframe vs. minicomputers vs. microcomputers); user interaction with dedicated systems vs. general purpose systems; computer-assisted technical writing.

B. Programming: operating systems - CP/M, UNIX; high level languages - BASIC, FORTRAN, PASCAL, C; assembly language.

C. Hardware Interfacing: digital logic; transducers; A/D and D/A converters; close-loop control.

D. Data Collection, Manipulation, and Display: ensemble averaging; digital smoothing; sampling theory; the Fourier transform; fast Fourier transform; apodization; aliasing; convolution and deconvolution; auto- and cross-correlation; data base management; graphics.

E. Numerical Methods: integration; solution of differential equations; linear algebra (e.g., matrix manipulations, linear equations solutions); combinatorics; pseudo-random number generation for Monte Carlo calculations; modeling and simulation (e.g., molecular dynamics, molecular conformational analysis); quantum chemistry; reaction dynamics; statistical mechanics.

F. Non-Numerical Methods: focus on abstract information-processing tasks; molecular structure representation; molecular model building; experimental design feasibility and optimization; pat-

tern recognition; searching of bibliographic and spectral data banks; substructure searching; applications of mathematical graph theory; expert knowledge-based artificial intelligence systems.

G. Graphics: function and data displays; interactive molecular structure display.

II. SAMPLE EXAMINATION QUESTIONS

The following questions are samples taken from examinations which have been given in college and university chemistry departments.

1. Define or explain the following terms: floating-point number system; inverted file; registration of chemical compounds; simplex; algorithm; heuristic; spline fit; Gaussian distribution.

2. Describe with several examples the Wiswesser linen notation (WLN) for representing chemical structures. Describe and give an example of a connection table representation of a chemical structure. What is the Morgan algorithm?

3. Illustrate how a first-order differential equation can be solved numerically.

4. How are random numbers generated by computers? Cite a source of truly random numbers from nature. What advantages do computer-generated random numbers have over truly random numbers?

5. What are the general properties of iterative numerical methods that are necessary to make them useful?

6. In "travelling salesman" problems, why is it necessary to search for adequate rather than optimal solutions?

7. Give the general form of the error function that is minimized in least squares curve fitting. How is it minimized? Is the result unique when a linear function is used? Why?

8. What is a chi-squared test, and how can it be used?

III. RESOURCE MATERIALS

The ACS Division of Computers in Chemistry organized and sponsored a symposium on computers in undergraduate chemistry. The proceedings are being published by Wiley-Interscience in 1984 under the title, "Computer Education of Chemists." Several of the chapters describe how colleges and universities have responded to the challenge of the rapid introduction and deployment of the computer in the undergraduate chemistry program.

INDUSTRIAL CHEMISTRY

(Prepared with the Help of the ACS Division of Chemical Education's Task Force on Academic Preparation and Industrial Careers in Chemistry)

The commercial practice of chemistry, in the chemical industry itself, and in the many associated industries, is a very important factor in our culture and in our economy. While the fundamental principles of this "industrial" chemistry are the same as "classical" chemistry, the practice of each is quite different. The differences result from basic differences in objectives. In the practice of industrial chemistry, the objective is to produce a product at a minimum total cost on a scale that will generate the maximum economic return. In the practice of classical chemistry in a typical academic laboratory, the objective is frequently to synthesize a substance in the most convenient manner in terms of the chemist's time and the laboratory equipment available. Because of these differences, the industrial chemist must not only be concerned with the fundamental principles of chemistry, but must also be concerned with such things as optimizing product yield and quality, minimizing material and process costs, while conforming to all pollution and safety standards.

I. The elements of industrial chemistry should be developed and practiced throughout the chemistry curriculum. However, courses in industrial chemistry have been found to be of great value in helping to organize the many different topics that the industrial chemist must deal with. A typical course in industrial chemistry should contain an introduction to the chemical industry and industrial practices, emphasizing the application of chemical principles to the development of comemrcial products and processes. The topics that should be included in a one-semester length course, along with a recommended time schedule are given in the following outline. In the absence of such a course, much of this material could be distributed through existing core courses.

WEEK

1 — 1. Industrial chemistry orientation - the economic importance and special characteristics of the chemical industry

2-3 — 2. Feedstocks, intermediates and products of the chemical industry; performance chemicals, commodities, specialities

Typical examples:

a. thermoplastics
b. thermosetting plastics
c. paints and coatings
d. elastomers
e. fibers
f. surfactants
g. pharmaceuticals
h. agricultural chemicals
i. paper
j. inorganic acids

3. Market demand, selling price, cost factors

4. Economics of scale

4 — 5. Research

a. market forecasts
b. product and patent relationships
c. information search and retrieval
d. regulation requirements
e. the choice of a route to the desired product
f. computer usage
g. new product decisions

5-9 6. Process chemistry

a. reaction types; batch continuous and semibatch relations
b. kinetics, experimental rate data
c. catalysis
d. process variables, optimization
e. scale-up consideration
f. environmental control, safety, hazards, government regulations

10-11 7. Material and energy balances

8. Heat transfer and energy sources

9. Fluid flow

10. Instrumentation and process control

12-13 11. Separation processes - criteria of selection

Typical example:

a. separation equilibria
b. distillation: azeotropes, steam
c. absorption
d. extraction
e. adsorption
f. crystallization
g. ion exchange
h. filtration

14 12. Process economics

a. cost factors
b. capital requirements
c. profit criteria
d. types of economic studies

13. Product development

a. application and testing
b. commercial development
c. technical service

15 14. Case studies illustrating the above topics and issues - preferably using personnel from local industries.

In addition to the exposures to industrial chemistry that are offered through the curriculum, it is recommended that summer and co-op jobs in the chemical industry be used to supplement the development of skills in the practice of industrial chemistry.

II. QUESTIONS ON INDUSTRIAL CHEMISTRY

1. Write chemical equations that show the preparations of the following commodity chemicals:

   a. Nylon precursors
   b. Polyester precursors
   c. Methacrylates
   d. Fatty alcohols
   e. Detergents
   f. Glycol

2. Why do factories discharge waste water that is not hot instead of using its energy content?

3. Explain the difference between a thermo-plastic and a thermo- setting material and explain why their processing conditions differ.

4. Why must silicon used in electronic devices be so pure?

5. Discuss the difference between toxic concentration and hazard; the concept of therapeutic index. Do all drugs have side effects? How, then, can they be used?

6. In chemical process diagrams how are reboilers represented?

7. Unlike laboratory distillations, many industrial separations feed the pre-heated stream into the column near the middle. Why?

8. The bromination of resorcinol gives three products in ratios which vary depending on the rate of stirring of the resorcinal solution during the addition of bromine. Explain.

9. In the commercial production of isopropyl benzene a large excess of benzene is reacted with propylene at a high temperature in a continuous vapor phase reaction over a fixed bed catalyst consisting of phosphoric acid on diatamaceous earth. Streams of propane are introduced at various points along the tubular reactor. Discuss how these conditions are consistent with the mechanism for this alkylation reaction and potential side reactions.

10. In a 250 ml trickle bed reactor packed with cation exchange resin in acid form and operated continuously, 60 g of propylene gas and 370 ml of distilled water are fed in a 1 hour period. Analysis of the feed gas indicated that it was 92% propylene and 8% propane. The reactor effluent consisted of 19.87 g of a non-condensable gas and 410 g of a liquid. Distillation of this liquid yielded 1.83 g of a liquid boiling at 68°C which was only slightly water soluble, and a 66.13 g fraction boiling at 80°C. This fraction was determined to be the isopropanol/water azeotrope which has a composition of 87.7% isopropanol by weight.

    a. Calculate the conversion of propylene, the yield of isopropanol based on propylene, and the selectivity of the catalyst.

b. What is the liquid boiling at 68°C? What is the % yield of this by-product?

11. Propylene oxide (methyl oxirane), an important commodity chemical, can be prepared by treating propylene chlorohydrin (1-chloro-2-propanol) with $Ca(OH)_2$. A minor (2-3%) product formed in this process is an ether.

Proposed a mechanism for its formation: $ClCH_2CH(CH_3)-O-CH(CH_3)CH_2Cl$.

12. There are problems with the process mentioned in question 11: chlorine is wasted, and there are environmental problems associated with disposal of large quantities of $CaCl_2$ solution contaminated with trace amounts of organics. A newer process involves oxygen transfer from an hydroperoxide. The most commonly mentioned hydroperoxides are derived from 2-methyl-propane (isobutane) or ethylbenzene. Why are thee compounds particularly suitable for hydroperoxide formation?

$$ROOH + CH_3CH{=}CH_2 \longrightarrow ROH + CH_3\underset{\diagdown\,O\,\diagup}{CH}\text{-}CH_2$$

13. What is the general use of cobalt and manganese soaps in organic chemistry?

14. Explain the terms heavy ends and raffinate.

15. Methyl methacrylate (NMA, methyl 2-methylpropenoic acid), the monomer used to make Plexiglas ™, is produced commercially from acetone cyanohydrin. Proposed a synthesis of MMA from acetone.

16. Trimethyloctadecylammonium chloride (1% in water) is sold as an antistatic agent for phonograph records. Suggest a synthesis of this material from the readily available (from animal fat) fatty acid stearic acid (octadecanoic acid).

17. Catalytic reforming, which converts n-alkanes of low octane number to high octane iso-alkanes, is an important refinery operation. Although the mechanism of this process is still under investigation, it is known that traces of HCl and alkenes are essential. Explain how these reagents could initiate rearrangement of butane.

$$CH_3CH_2CH_2CH_3 \xrightarrow[\text{Pt catalyst}]{300\text{-}400\ ^{o}C} CH_3\underset{CH_3}{CH}CH_3$$
traces of C=C +HCl

INORGANIC CHEMISTRY

(Prepared with the Help of the ACS Division of Inorganic Chemistry)

I. Introductory Inorganic Course

A. Periodicity: basis in atomic structure; classification of the elements; trends in oxidation states, radii, electronegativity; diagonal relationships; term symbols for atomic ground states.

B. Ionic Interactions: close packed systems; crystal lattices; Born-Haber cycles (lattice energy calculations); ionic radii.

C. Systematics of the Chemistry of the Elements: alkalies, alkaline earths, halogens, chalcogens, pnicogens, noble gases, carbon group, boron group, transition elements, lanthanides, actinides.

D. Acid-Base Chemistry and Non-Aqueous Solvents: acid-base concepts, hard and soft acids and bases, non-aqueous solven systems.

II. Post-Introductory Course - Post First Half of Physical Chemistry

A. Bonding and Structure: VSEPR theory, symmetry, LCAO-MO theory, valence bond theory, hybridization, bond energies, covalent radii.

B. Coordination Chemistry: stereochemistry and isomerism, bonding (valence bond, ligand field, and MO), magnetic and spectroscopic properties, synthesis, reaction mechanisms, redox chemistry, metal-metal bonds, metal clusters.

C. Solid State Chemistry: simple metals (structure and bonding), semiconductors, band theory (free electron and tight binding viewpoints), transition metal ions in lattices (spinels), non-stoichiometric solids.

D. Organometallic Chemistry: EAN rule; carbonyls and nitrosyls; olefin, acetylene, alkyl, arene complexes; metallocenes; oxidative addition and reductive elimination; fluxionality; homogeneous catalysis; organometallic clusters.

III. Below are selected special topics. As many of these topics as possible should be covered in the time available.

A. Bioinorganic Chemistry: metalloporphyrins, vitamin B_{12} and cobalamines, nitrogen fixation, metalloenzymes, non-metallic bioinorganic chemistry.

B. Inorganic Environmental Chemistry.

C. Boranes.

D. Inorganic Ring Systems and Polymers: silicates, sulfur nitrides.

IV. LABORATORY COURSE - Concurrent with Post Introductory Inorganic Course

A selection of syntheses are listed below which demonstrate chemical principles discussed in the above courses. Incorporated into these experiments are a variety of techniques currently used by inorganic chemists and a range of inorganic materials.

Syntheses	Techniques
$K_2S_2O_8$	Electrolysis
Me_3NBF_3	Vacuum manipulation, IR
$NaNH_2$	Non-aqueous solvent
$CrCl_3(THF)_3$	Inert atmosphere box, Soxhlet extractor
$Ni[P(OMe)_3]_4$ olefin isomerization catalyst	Gas chromatography
Sm_2O_3; Nd_2O_3, Pr_6O_{11}	Ion exchange
$Co_2(CO)_8$	Autoclave, IR
$[Co(NH_3)_5Cl]^{2+}$ for aquation kinetics	UV-visible
$[Co\ en_3]^{+3}$ for optical resolution	Optical rotations
$[Ni(glycinate)_n]^{(2-n)+}$ for successive K_{stab} measurement	pH measurements
$(\eta^6\text{-}C_6H_6)\ Cr(CO)_3$	IR, NMR, mass spectra, autoclave
$(\eta^5\text{-}C_5H_5)_2$ Fe and derivatives	TLC and column chromatography
$[Cr(NH_3)_6](NO_3)_3$	Magnetic susceptibility
$[M_6Cl_{12}]^{n+}$ cluster (M = Ta or Nb)	Dry box technique, high temperature synthesis
ZnS	High temperature transport synthesis
FeF_6^{-3}, $Fe(CN)_6^{-3}$	Paramagnetic susceptibility bn NMR
$[Re_2Cl_8]^{-2}$	IR, UV-visible

V. SAMPLE PERFORMANCE OBJECTIVES for the core lecture courses. (Most are taken from the 1978 report of the Curriculum Committee of the Division of Chemical Education).

Periodicity:

1. Define the following with the aid of a suitable example:
   a. an eigenvalue
   b. ionization energy
   c. a node
   d. penetration effects
   e. Zeeman effect
   f. shielding or screening
2. Indicate the expected variation in properties such as the following as one crosses a given period.
   a. covalent radius
   b. electronegativity
   c. ionization energy
   d. electron affinities
   e. natural abundance
3. Arrange a given set of fluorides (as as InF_3, CF_4, BeF_2, TeF_6, SbF_5) in order of increasing ionic character.

Ionic Interactions:

4. List the thermodynamic quantities necessary to construct a Born-Haber cycle for the formation of an ionic compound from its elements.
5. Given the ion radii of a cation and an anion, calculate their radius ratio and make a theoretical prediction of the crystalline lattice they will form.

Systematics of the Chemistry of the Elements:

6. Arrange a set of reagents [such as Br_2, $(CN)_2$, F_2, I_2, $(SCN)_2$] in the expected order of oxidizing ability.
7. Discuss the relative stability, molecular formulas, and structure of interhalogen compounds in terms of the nature of the halogens involved.

Acid-Base Chemistry and Non-Aqueous Solvents:

8. Select the stronger acid from pairs such as $B(CH_3)_3$, BCl_3; $B(CH_3)_3$, $B(i\text{-}C_3H_7)_3$; etc.
9. Define the leveling effect.

Bonding and Structure:

10. By way of a M.O. energy level diagram show the interaction of metal d, s, and p orbitals with a σ set of ligand orbitals in an octahedral field.
11. Define the following with the aid of a suitable example: (a) Lewis structure; (b) valence atomic orbital; (c) bonding molecular orbital; (d) antibonding molecular orbital; (e) non-bonding molecular orbital; (f) localized molecular orbital; (g) delocalized molecular orbital; (h) homonuclear; (i) heteronuclear; (j) resonance; (k) lone pair; (l) sigma bond; (m) pi bond; (n) delta bond; (o) Bent's Rule; (p) electronegativity; (q) partial ionic character; (r) effective nuclear charge; (s) net bond order; (t) double bond; (u) triple bond; dipole moment; (w) covalent radius; (x) ionic radius; (y) Van der Waals radius; (z) sp^2 hybrid orbitals; (aa) sp^3 hybrid orbitals; (bb) sp^3d hybrid orbitals; (cc) sp^3d^2 hybrid orbitals.

Coordination Chemistry:

12. Stereoisomers:
    a. Given the following complexes, predict the possibility of stereoisomerism: tetrahedral and square planar MA_2B_2; square planar $M(CD)_2$; where CD represents an unsymmetrical bidentate ligand such as $NH_2CH_2CH_2PH_2$.

b. Given the octahedral complex $MA_2B_2C_2$, draw structures of all possible stereoisomers. Are these isomers optically active?

Applications of Crystal Field Theory:

13. Given the expected relative magnitude of the radii of metal ions M^{+q}: $d^1 > d^2 > d^3 > d^4 > d^5$ in the gas phase, explain the "anomalous" order of the observed radii in crystals and complexes, and the "anomalous" order of hydration energies, in terms of crystal field theory.

Synthesis and Reactions

14. a. Describe the procedure for the synthesis of $Co(NH_3)_6^{3+}$ and explain the function of the catalyst which is employed.
    b. Give examples of substitution labile cobalt and platinum complexes.
    c. Give an example reaction for an inner sphere redox reaction and of an outer sphere redox reaction.

Solid State Chemistry

15. Define, in terms of metallic bond theory, insulator, conductor, intrinsic and extrinsic semi-conductor, and p and n-type semi-conductors.
16. List 2 factors that control the solubility of one metal in another.
17. Compare the spectral, magnetic, and structural properties of the three Robin and Day classes of mixed oxidation state solids.

Organmetallic Chemistry:

18. Given an example of the application of Gilman's displacement rule in the preparation of a main-group organometallic.
19. Give the steps in homogeneous catalysis reaction wherein the catalyst is an organometallic compound.

Bioinorganic Chemistry:

20. List three nonmetals (excluding C, H, O, and N) that are essential to life and briefly indicate (50 words) one biological function of each.
21. Give an example of the application of the principles of hard and soft acids and bases to the poisoning of enzymes by heavy metal ions and the reversal by agents containing thiol groups (-SH).

Inorganic Environmental Chemistry:

22. Give two examples of the reduction in toxicity of a metal or a ligand via complexation.
23. Boranes: Give laboratory syntheses for B_2H_6 and BH_4^-.

Inorganic Ring Systems and Polymers:

24. Give laboratory preparations for $(PNCl)_3$, $B_3N_3H_6$, and Na_3O_9.
25. Draw structures for polymers of the silicate, phosphonitrilic, phosphate and sulfur nitride types.

ORGANIC CHEMISTRY

(Prepared with the Help of the ACS Division of Organic Chemistry)

I. A chemistry major course in organic chemistry should provide a thorough grounding in the following topics:

A. General Aspects of Structure - including bonding concepts, molecular architecture, isomerism (structural, conformational, stereo), and nonmenclature.

B. Correlation of Physical Properties and Molecular Structure - including UV/Vis, IR, ^{1}H-NMR, ^{13}C-NMR, and mass spectra.

C. Correlation of Chemical Reactivity and Molecular Structure - including acid and base phenomena, electronic effects, and steric effects.

D. Reaction Mechanisms - including nucleophilic and electrophilic substitution, electrophilic addition, elimination, carbonyl addition, free radical substitution and addition, oxidation and reduction, and molecular rearrangements.

E. Chemical Kinetics - including a brief introduction to 1st order and 2nd order reaction kinetics, thermodynamic parameters, and activation parameters.

F. Detailed Consideration of Specific Classes of "Simple" Compounds - including alkanes, alkenes, alkynes, arenes, halides, alcohols and phenols, ethers, amines, aldehydes, ketones, carboxylic acids, and carboxylic acid derivatives.

G. Detailed Consideration of Specific Classes of Polyfunctional Molecules - including α,β-unsaturated carbonyl compounds, polyenes, dicarbonyl compounds (including quinones), hydroxy acids, and amino acids.

H. Detailed Consideration of Specific Classes of "Complex" Compounds - including saccharides and polysaccharides, amino acids and polypeptides, nucleic acids and polynucleotides, acetogenins, alkaloids, and vitamins.

I. Organic Synthesis - including moderately challenging "sequence syntheses".

II. In addition to the topics listed above, a chemistry major course should give some attention to the historical aspects of organic chemistry, the organic chemistry of polymers, the biochemical relationships of organic molecules, and the industrial ramifications of organic processes.

III. For courses seeking the level of sophistication reflected by several of the "big" textbooks currently available some selection among the following topics might also be included.

A. Additional Discussion of Stereochemistry

B. Additional Discussion of Spectroscopy

C. Additional Discussion of Organometallic Chemistry

D. Photochemistry

E. Thermal Rearrangements and Cycloaddition Reactions

F. Orbital Symmetry Considerations

G. Heterocyclic Chemistry

H. Nonbenzenoid Aromatic Compounds

I. Natural Product Synthesis

IV. The laboratory associated with the chemistry major course in organic chemistry should provide a thorough grounding in the following experimental techniques:

A. Isolation and Purification Techniques - including extraction, distillation, sublimation, crystallization, and chromatography (column, thin layer, gas-liquid, HPLC).

B. Analytical Techniques - including chromatography (see above) and spectrophotometry (UV/Vis, IR, NMR, mass spectra).

C. Synthesis Techniques - including the synthesis of an appropriately selected group of "simple" organic compounds.

D. Identification Techniques - including the application of analytical techniques (see above) and synthesis techniques (see above) to the identification of appropriately chosen "unknown" compounds.

E. Library Techniques - including instruction in how to locate information pertinent to organic analysis and synthesis in the library.

V. It is recommended that the laboratory material traditionally comprising the advanced course called "Qualitative Organic Analysis" be incorporated into the second semester of the two-semester laboratory sequence associated with the major course in organic chemistry. An advanced laboratory course in organic chemistry might then be devoted to modern methods of organic synthesis (e.g. multi-step syntheses) and be designed as an introduction to modern methods of organic chemical research.

POLYMER CHEMISTRY

(Prepared with the Help of the ACS Division of Polymer Chemistry)

The chemistry of polymers should be developed throughout the chemistry curriculum. Below are sample topics and questions for core course. Major topics include morphology, molecular weights, kinetics of polymerization. Supplementary topics include viscoelastic properties, solubility, natural and biomedical polymers, additives, polymer technology, monomer synthesis.

Some topics which should be integrated, at appropriate points, throughout the courses listed:

IA. General Chemistry

Classroom time - should include illustrations and use of polymers in calculations such as - the repeat unit of polystyrene is $[CH_2CH(C_6H_5)]$, what is the % C and % H. Topics to be covered - Macromolecules - definition; importance - all about us; basis for plant and animal life. Rubbers (elastomers), fibers & plastics - examples; uses: thermosetting, thermoplastic - definition, examples. Common polymers - structural unit; uses: polystyrene, polyethylene, polysaccharides, nylons, polyesters, nucleic acids, proteins, polyvinyl chloride. Inorganic polymers - glass, concrete, diamonds, graphite. Typical properties - memory, solubility, viscous solutions. Polymers as tools for delivering necessary concepts: a. importance of shape & chemical nature; mode of linkage-polysaccharides, -cis-trans for isoprene; sequence & shape - enzymes, proteins, nucleic acids; b. need to utilize renewable resources; c. importance of chemical industry; d. thermochemistry - importance in industrial scale syntheses; e. importance of synthetic (paints, clothing, electronics, etc.) and nature (skin, hair, wool, paper, wood, etc.) materials in our lives; f. importance of secondary and primary bonding (such as ethylene being a gas, paraffins as waxes, and polyethylene a solid).

B. General Chemistry Questions

1. What is the ratio of ethylene (C_2H_4) mers to vinyl chloride (C_2H_3Cl) mers in a copolymer of the two that is by weight 24% chlorine?

2. Heated, molten sulfur becomes increasingly dark and, to a point, more viscous, owing to (a) ring-breaking to form puckered S_8 rings (c) ring-breaking to form polymers with radical ends (d) radical uncoiling of linear polymers. Select one.

3. The viscosity of 10-W-40 motor oil varies more slowly with temperature than that of regular motor oil because it contains (a) a silicone additive that reduces the activation energy of viscous flow (b) a boron additive that increases the degree of polymerization of branched hydrocarbons (c) a polymer additive that uncoils with increasing temperature (d) only unbranched hydrocarbons with even numbers of carbon atoms. Select one.

IIA. Organic Chemistry

1. Extension of following to include polymers - addition reactions (e.g. free radical, anionic, cationic), condensation reactions, (e.g. esterification, amidation), ring opening (e.g. lactams, lactones).

2. Structure & synthesis of polychloroprene, polycarbonates, polyacetals, polyacrylonitrile, polyamides, polyesters, polyethylene, polyvinyl chloride, polyvinyl alcohol, polyisobutylene, polymethyl methacrylate, polystyrene, polytetrafluoroethylene, polyethers.

3. Polymeric nature of natural polymers as polysaccharides, proteins, enzymes, nucleic acids including secondary and tertiary structures.

4. Kinetics of step and chain processes related to polymerization.

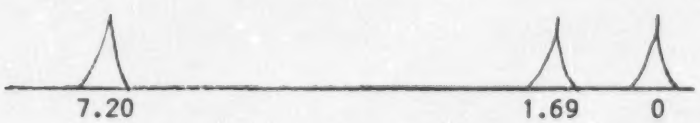
5. Molecular weight and molecular weight distribution, stereoregular polymers and their catalysts, crosslinking, structure-property relationships (as in elastomers, fibers, and plastics), head-to-tail preferred structure, copolymers. Terms: endgroup termination, plasticizer, oligomer, thermoplastic, thermoset, amorphous, crystalline, backbone, branching, random copolymer, block copolymer, alternating copolymer.

B. Organic Chemistry Questions

1. Draw the repeat unit obtained in condensation polyerization of $HOOC(CH_2)_6COOH$ AND $H_2N\ (CH_2)_4NH_2$.

2. Which is most likely to polymerize by anionic initiation?
(a) $H_2C{=}CHCN$ (b) $H_2C{=}CHCl$ (c) $H_2C{=}CHOCH_3$ (d) $F_2C{=}CF_2$

3. A polymer dissolved in $CDCl_3$ gives this 60 MHz NMR spectrum.



The polymer is (a) polystyrene (b) poly (methacrylic acid) (c) bisphenol-A-carbonate (d) poly (vinyl alcohol) (e) butadiene -styrene rubber.

IIIA. Physical

1. Polymers as tools for delivering necessary concepts: gases (ideal gas compared to ideal rubber), quantization and statistics (configuration of flexible polymer chains in solution, thermodynamics and thermochemistry of polymerizations and polymer solubility), phase equilibrium (polymer molecular weight fractionation), solids

(polymer crystallization, crystallinity and amorphous fraction), liquids (rheology, polymer solubility and viscosity), kinetics (step growth, chain growth, and enzyme kinetics), catalysis (control of regularity).

2. Polymer topics: comparison of property-structure properties, molecular weight and its distributions and determinations (light scattering, ultracentrifugation, fractionation techniques including GPC, osmometry, viscometry), glass and melting transitions, property behavior and models, polymer solubility.

B. Physical Chemistry Questions

1. If polymerization is stopped after only a few percent of monomer is converted to polymer, the polymer's molecular weight, compared to that for a higher percent polymerization, will be for

chain polymerization	and	condensation polymerization
low		low
low		high
high		low
high		high

independent of percent monomer polymerized

2. Which technique is NOT used to determine polymer molecular weights? (a) Vapor pressure osmometry (b) electron microscopy (c) gel permeation chromatography (d) thermogravimetric analysis (e) dilute solution viscosity.

3. Globular polymers (a) have an effect on intrinsic viscosity independent of their molecular weight (b) show more flow birefringence than random coil polymers (c) are more likely to be found in ideal solvents than are random coil polymers (d) are usually extensively hydrogen-bonded by the solvent.

IVA. Inorganic Chemistry

1. Polymer nature of silicones, phosphazenes, polysulfides, silicates, polyphosphates, and borazenes.

2. Catalytic systems important to polymerization processes of organic monomers: Zeigler catalysts, metal alkyls, and anchored metal catalysts.

3. Solid state structure of inorganic polymers, e.g.: oxides, sulfides, carbon (graphite & diamond).

4. Additional polymers: aluminum hydride/alkoxide, $(SO_3)_x$, sulfur, phosphorus, R_2Sn0.

B. Inorganic Chemistry Questions

1. Discuss the bonding in the lubricant MoS_2.

2. Sketch structures and give empirical formulas for single-chain, double-chain, and sheet silicates.

3. Select the single, best phrase given that describes the bonding in the following inorganic polymers.

$(PNCl_2)_x$	____ 1.	Sheet structure with sigma-bonded network reinforced by π bonding.
$(Mg_2B_2)_x$	____ 2.	Lewis acid-base bonded backbone.
$(SN)_x$	____ 3.	Sigma framework enforced by d-p π bonding.
$(SO_3)_x$	____ 4.	Shared corners, edges, and/or faces of octahedra and tetrahedra.
$PW_{12}O_{40}^{3-}$	____ 5.	Chain structure with one-dimensional metal-like electron delocalization.
$(BN)_x$	____ 6.	Three-centered bonding in bridges.

4. Outline a mechanism for Ziegler-Natta polymerization of ethylene by a heterogeneous Ti(III) catalyst.

VA. Analytical

1. Analytical techniques applicable to smaller molecules are typically applicable to the analysis of polymeric materials with little or no change (includes electronic, spectroscopic, and thermal techniques).

2. Application of polymers in analytical chemistry, including: stationary phases in chromatography (e.g. silica, alumina), membranes in osmometry (e.g. cellulose derivatives), and selective electrodes (e.g. enzymes).

3. Special techniques applicable to polymers including the following: molecular weight determination techniques (light scattering, ultra centrifugation, membrane, endgroup determinations, viscometry); molecular weight distribution techniques (GPC and other fractionation techniques).

4. Selected laboratory analyses employing polymeric materials, such as: elemental analysis (Cl analysis of polyvinyl chloride), and molecular weight determination (endgroup employing Carbowax).

Polymer Course. Information and a suggested syllabus can be obtained from Jane C. Vogl, Polymer Division Business Office Manager, Polytechnic Institute of New York, 333 Jay Street, Brooklyn, N.Y., 11201.